10/030,436

=> d his

(FILE 'HOME' ENTERED AT 12:24:22 ON 07 JUN 2004)

FILE 'REGISTRY' ENTERED AT 12:24:37 ON 07 JUN 2004
L1 STRUCTURE UPLOADED
L2 QUE L1
L3 42 S L2
L4 611 S L2 SSS FUL

FILE 'CAPLUS' ENTERED AT 12:25:01 ON 07 JUN 2004
L5 267 S L4
L6 ANALYZE L5 1- RN HIT : 608 TERMS

FILE 'REGISTRY' ENTERED AT 12:25:23 ON 07 JUN 2004
L7 1 S 102771-26-6/RN
L8 1 S 161832-65-1/RN
L9 1 S 143692-48-2/RN
L10 1 S 161832-71-9/RN
L11 STRUCTURE UPLOADED
L12 QUE L11
L13 53 S L12 SUB=L4 FUL
L14 558 S L4 NOT L13
L15 STRUCTURE UPLOADED
L16 QUE L15
L17 562 S L16 SUB=L4 FUL
L18 558 S L17 NOT (L7 OR L8 OR L9 OR L10)

FILE 'CAPLUS' ENTERED AT 12:29:49 ON 07 JUN 2004
L19 73 S L18
L20 8 S L13

=> d l2
L2 HAS NO ANSWERS
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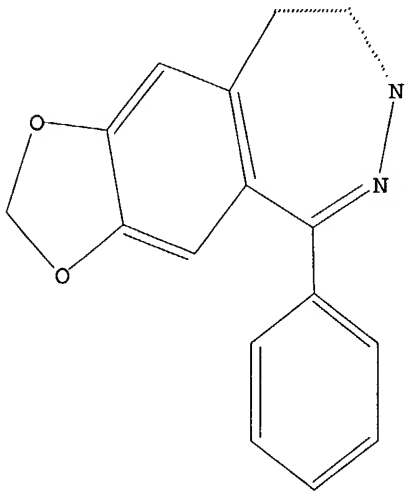

Structure attributes must be viewed using STN Express query preparation.
L2 QUE ABB=ON PLU=ON L1

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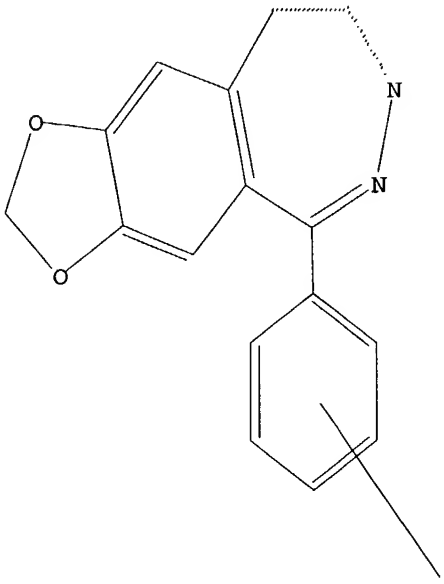
L11 STR



Structure attributes must be viewed using STN Express query preparation.
L12 QUE ABB=ON PLU=ON L11

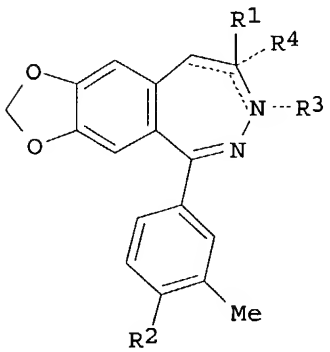
=> d ibib abs hitstr l20 1-8

applicant

L20 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:50649 CAPLUS
DOCUMENT NUMBER: 134:100896
TITLE: Preparation of new 1,3-dioxolo[4,5-h][2,3]benzodiazepines as neuroprotective agents
INVENTOR(S): Greff, Zoltan; Szabo, Geza; Barkoczy, Jozsef; Ratkai, Zoltan; Blasko, Gabor; Simig, Gyula; Gigler, Gabor; Martonne Marko, Bernadett; Levay, Gyorgy; Tihanyi, Karoly; Egyed, Andras; Simo, Annamaria
PATENT ASSIGNEE(S): Egis Gyogyszergyar Rt., Hung.
SOURCE: PCT Int. Appl., 80 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001004122	A2	20010118	WO 2000-HU74	20000704
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1200442	A1	20020502	EP 2000-944129	20000704
EP 1200442	B1	20030625		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003504372	T2	20030204	JP 2001-509731	20000704
AT 243699	E	20030715	AT 2000-944129	20000704
BG 106281	A	20030131	BG 2002-106281	20020107

PRIORITY APPLN. INFO.: HU 1999-2291 A 19990707
WO 2000-HU74 W 20000704
OTHER SOURCE(S): MARPAT 134:100896
GI



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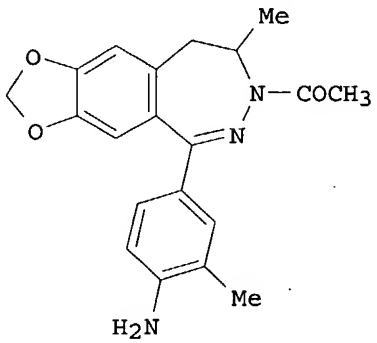


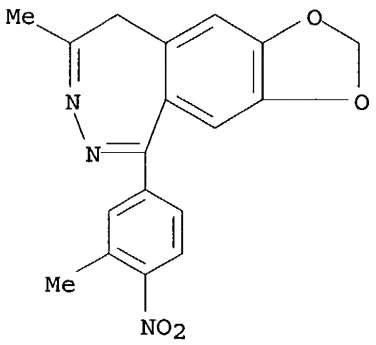
II

AB The title compds. [I; R1 = Me, CHO, CO2H, etc.; R2 = NO2, NH2; R3 = H, alkanoyl, CONR7R8 (wherein R7, R8 = H, alkoxy, alkyl, cycloalkyl; NR7R8 =

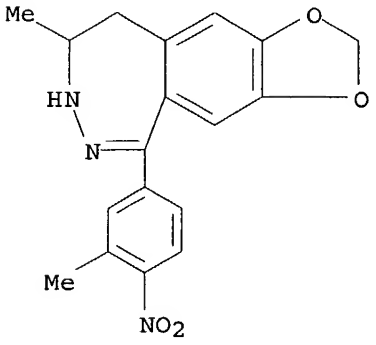
(un)saturated 5-6 membered heterocyclic ring optionally containing one or more further N, S and/or O atom(s)); R4 = H, alkyl; the dotted lines have the following meaning: if R3 and R4 are not present, the bond between positions C8 and C9 is a single bond and the bond between positions C8 and N7 is a double bond; if R3 and R4 are present, the bonds between positions C8 and C9 and between position C8 and N7 are single bonds; and if R3 is present and R4 is missing, the bond between positions C8 and C9 is a double bond and the bond between positions C8 and N7 is a single bond] which have neuroprotective effect, were prepared E.g., a multi-step synthesis of 1,3-dioxolo[4,5-h][2,3]benzodiazepine II which showed PD50 (the dose that prolonged survival by 50%) of 5.4 mg/kg in MgCl2-induced global cerebral ischemia in mice (i.p.), was given.

IT **319907-43-2P 319907-44-3P 319907-50-1P 319907-51-2P 319907-52-3P 319907-53-4P 319907-60-3P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of new 1,3-dioxolo[4,5-h][2,3]benzodiazepines as neuroprotective agents)

RN 319907-43-2 CAPLUS
CN 9H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine, 8-methyl-5-(3-methyl-4-nitrophenyl)- (9CI) (CA INDEX NAME)

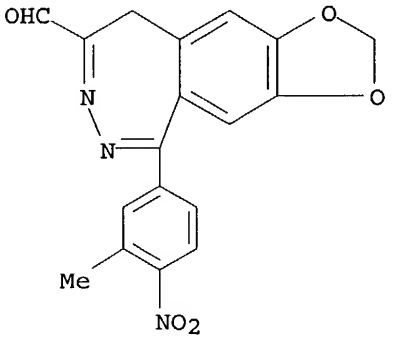


RN 319907-44-3 CAPLUS
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine, 8,9-dihydro-8-methyl-5-(3-methyl-4-nitrophenyl)- (9CI) (CA INDEX NAME)

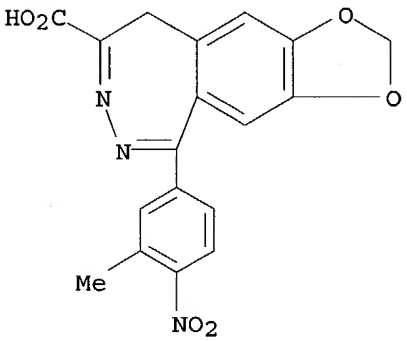


RN 319907-50-1 CAPLUS

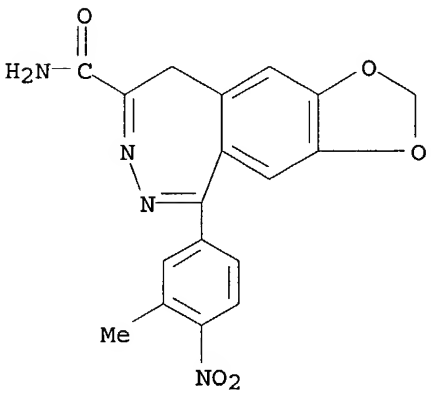
CN 9H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine-8-carboxaldehyde, 5-(3-methyl-4-nitrophenyl)- (9CI) (CA INDEX NAME)



RN 319907-51-2 CAPLUS
CN 9H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine-8-carboxylic acid, 5-(3-methyl-4-nitrophenyl)- (9CI) (CA INDEX NAME)

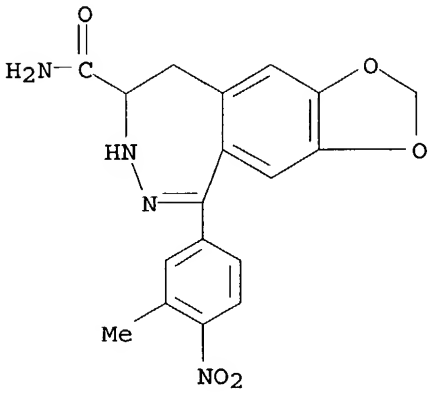


RN 319907-52-3 CAPLUS
CN 9H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine-8-carboxamide, 5-(3-methyl-4-nitrophenyl)- (9CI) (CA INDEX NAME)

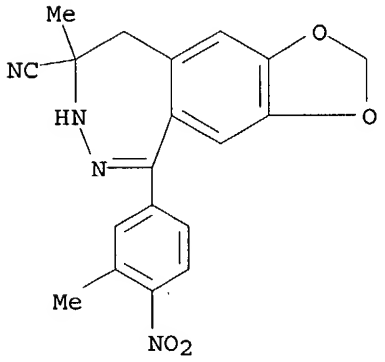


RN 319907-53-4 CAPLUS
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine-8-carboxamide,

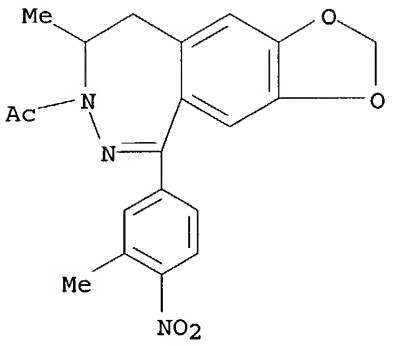
8,9-dihydro-5-(3-methyl-4-nitrophenyl)- (9CI) (CA INDEX NAME)



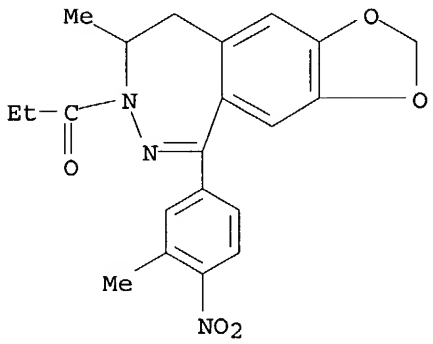
RN 319907-60-3 CAPLUS
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine-8-carbonitrile,
8,9-dihydro-8-methyl-5-(3-methyl-4-nitrophenyl)- (9CI) (CA INDEX NAME)



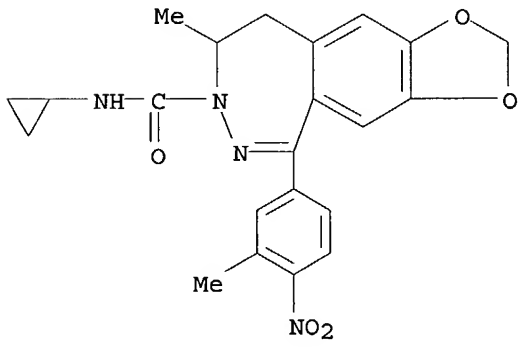
IT **319907-45-4P 319907-46-5P 319907-47-6P**
319907-48-7P 319907-49-8P 319907-54-5P
319907-55-6P 319907-56-7P 319907-57-8P
319907-58-9P 319907-59-0P 319907-61-4P
319907-62-5P 319907-63-6P 319907-64-7P
319907-65-8P 319907-66-9P 319907-67-0P
319907-69-2P 319907-70-5P 319907-71-6P
319907-72-7P 319907-73-8P 319907-74-9P
319907-75-0P 319907-76-1P 319907-77-2P
319907-78-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of new 1,3-dioxolo[4,5-h][2,3]benzodiazepines as neuroprotective agents)
RN 319907-45-4 CAPLUS
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine, 7-acetyl-8,9-dihydro-8-methyl-5-(3-methyl-4-nitrophenyl)- (9CI) (CA INDEX NAME)



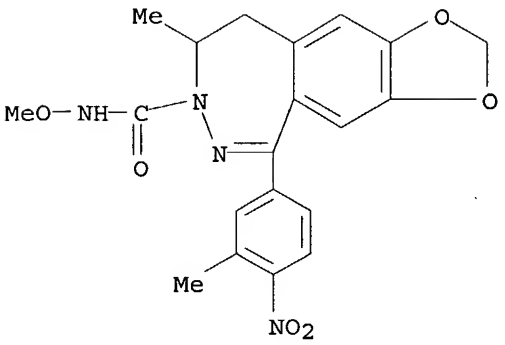
RN 319907-46-5 CAPLUS
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine, 8,9-dihydro-8-methyl-5-(3-methyl-4-nitrophenyl)-7-(1-oxopropyl)- (9CI) (CA INDEX NAME)



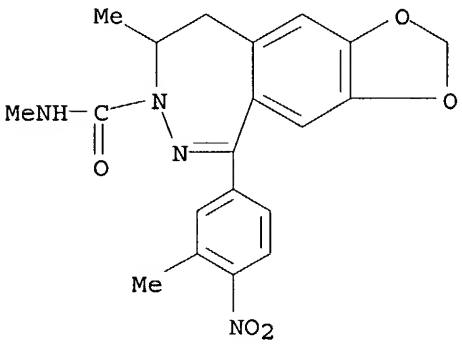
RN 319907-47-6 CAPLUS
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine-7-carboxamide, N-cyclopropyl-8,9-dihydro-8-methyl-5-(3-methyl-4-nitrophenyl)- (9CI) (CA INDEX NAME)



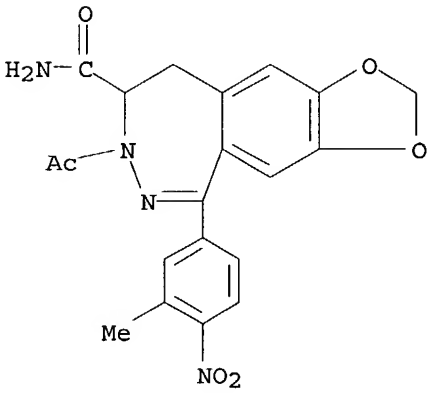
RN 319907-48-7 CAPLUS
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine-7-carboxamide, 8,9-dihydro-N-methoxy-8-methyl-5-(3-methyl-4-nitrophenyl)- (9CI) (CA INDEX NAME)



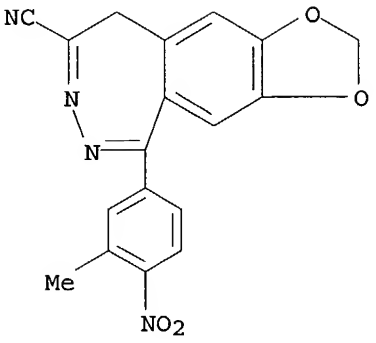
RN 319907-49-8 CAPLUS
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine-7-carboxamide, 8,9-dihydro-N,8-dimethyl-5-(3-methyl-4-nitrophenyl)- (9CI) (CA INDEX NAME)



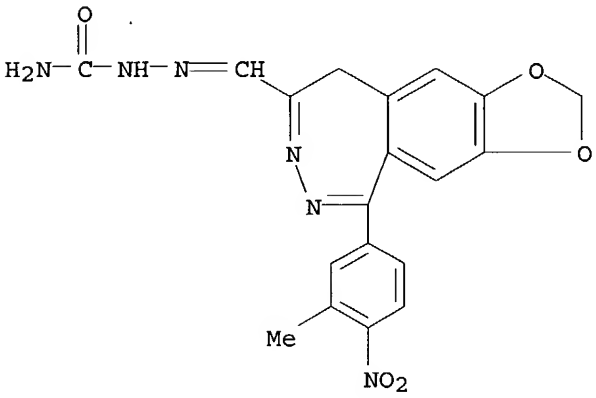
RN 319907-54-5 CAPLUS
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine-8-carboxamide, 7-acetyl-8,9-dihydro-5-(3-methyl-4-nitrophenyl)- (9CI) (CA INDEX NAME)



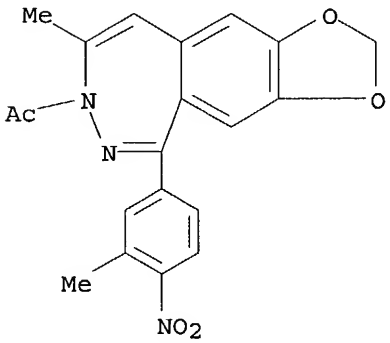
RN 319907-55-6 CAPLUS
CN 9H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine-8-carbonitrile, 5-(3-methyl-4-nitrophenyl)- (9CI) (CA INDEX NAME)



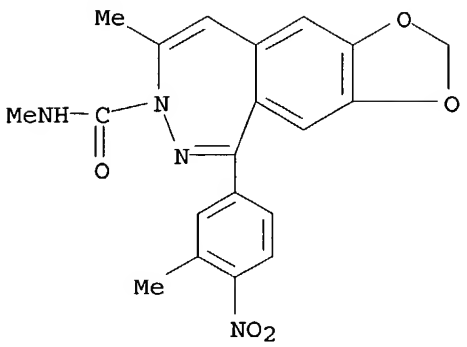
RN 319907-56-7 CAPLUS
CN Hydrazinecarboxamide, 2-[[5-(3-methyl-4-nitrophenyl)-9H-1,3-dioxolo[4,5-h][2,3]benzodiazepin-8-yl]methylene]- (9CI) (CA INDEX NAME)



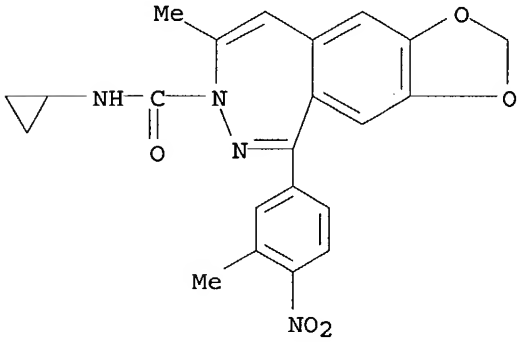
RN 319907-57-8 CAPLUS
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine, 7-acetyl-8-methyl-5-(3-methyl-4-nitrophenyl)- (9CI) (CA INDEX NAME)



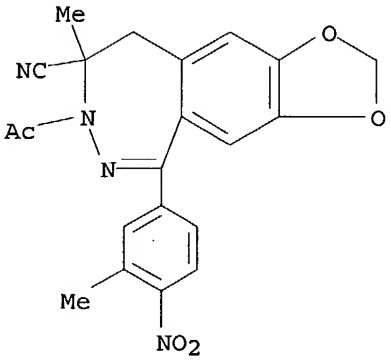
RN 319907-58-9 CAPLUS
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine-7-carboxamide, N,8-dimethyl-5-(3-methyl-4-nitrophenyl)- (9CI) (CA INDEX NAME)



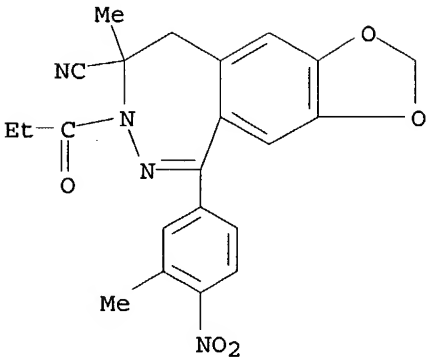
RN 319907-59-0 CAPLUS
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine-7-carboxamide, N-cyclopropyl-8-methyl-5-(3-methyl-4-nitrophenyl)- (9CI) (CA INDEX NAME)



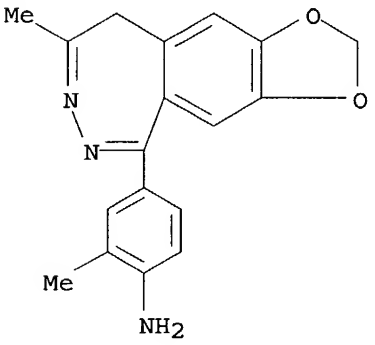
RN 319907-61-4 CAPLUS
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine-8-carbonitrile, 7-acetyl-8,9-dihydro-8-methyl-5-(3-methyl-4-nitrophenyl)- (9CI) (CA INDEX NAME)



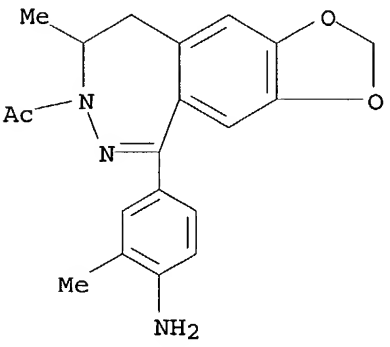
RN 319907-62-5 CAPLUS
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine-8-carbonitrile, 8,9-dihydro-8-methyl-5-(3-methyl-4-nitrophenyl)-7-(1-oxopropyl)- (9CI) (CA INDEX NAME)



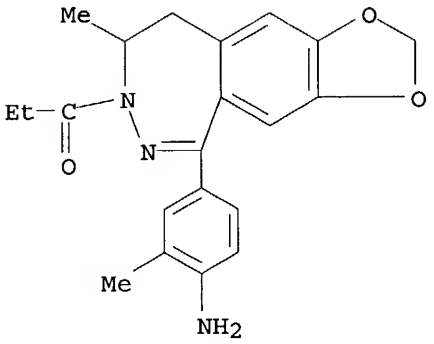
RN 319907-63-6 CAPLUS
CN Benzenamine, 2-methyl-4-(8-methyl-9H-1,3-dioxolo[4,5-h][2,3]benzodiazepin-5-yl)- (9CI) (CA INDEX NAME)



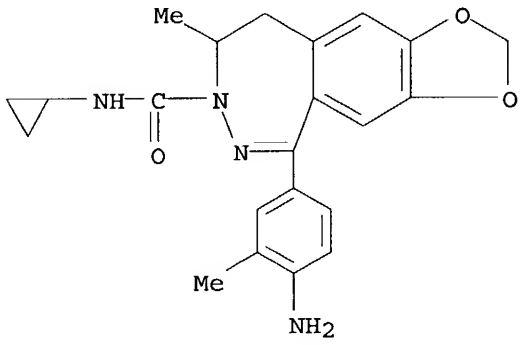
RN 319907-64-7 CAPLUS
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine, 7-acetyl-5-(4-amino-3-methylphenyl)-8,9-dihydro-8-methyl- (9CI) (CA INDEX NAME)



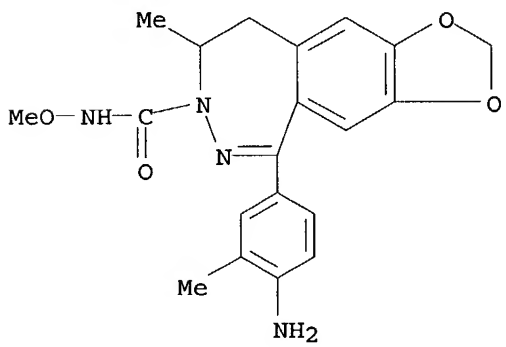
RN 319907-65-8 CAPLUS
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine, 5-(4-amino-3-methylphenyl)-8,9-dihydro-8-methyl-7-(1-oxopropyl)- (9CI) (CA INDEX NAME)



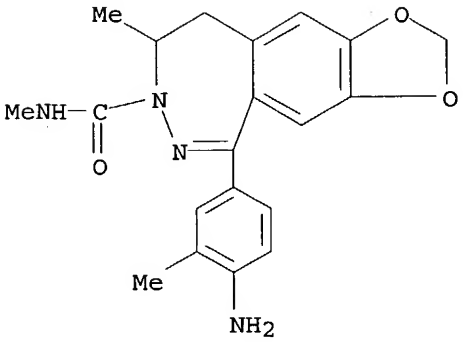
RN 319907-66-9 CAPLUS
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine-7-carboxamide, 5-(4-amino-3-methylphenyl)-N-cyclopropyl-8,9-dihydro-8-methyl- (9CI) (CA INDEX NAME)



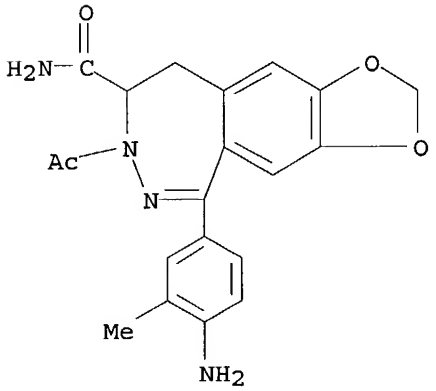
RN 319907-67-0 CAPLUS
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine-7-carboxamide, 5-(4-amino-3-methylphenyl)-8,9-dihydro-N-methoxy-8-methyl- (9CI) (CA INDEX NAME)



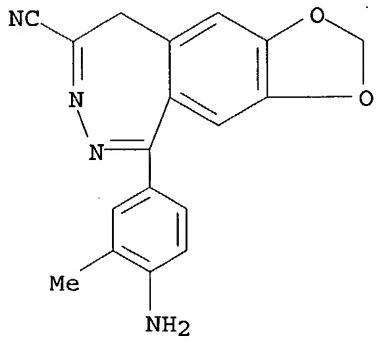
RN 319907-69-2 CAPLUS
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine-7-carboxamide, 5-(4-amino-3-methylphenyl)-8,9-dihydro-N,8-dimethyl- (9CI) (CA INDEX NAME)



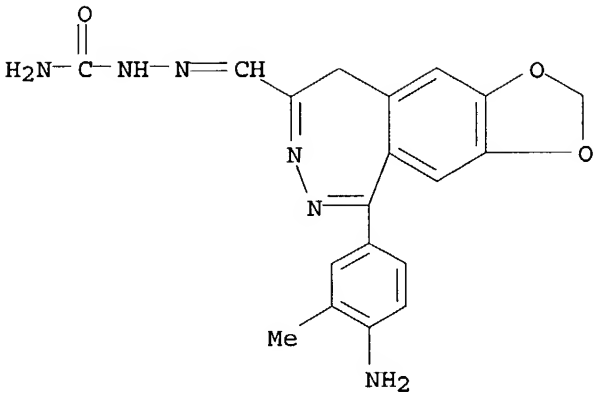
RN 319907-70-5 CAPLUS
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine-8-carboxamide, 7-acetyl-5-(4-amino-3-methylphenyl)-8,9-dihydro- (9CI) (CA INDEX NAME)



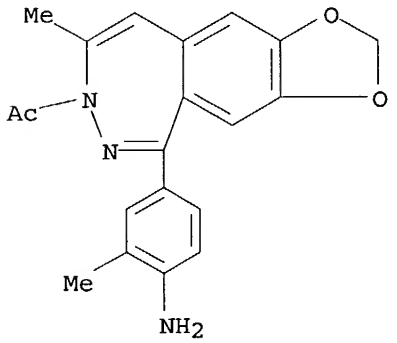
RN 319907-71-6 CAPLUS
CN 9H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine-8-carbonitrile, 5-(4-amino-3-methylphenyl)- (9CI) (CA INDEX NAME)



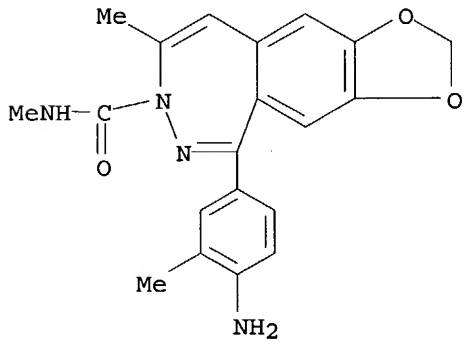
RN 319907-72-7 CAPLUS
CN Hydrazinecarboxamide, 2-[[5-(4-amino-3-methylphenyl)-9H-1,3-dioxolo[4,5-h][2,3]benzodiazepin-8-yl]methylene]- (9CI) (CA INDEX NAME)



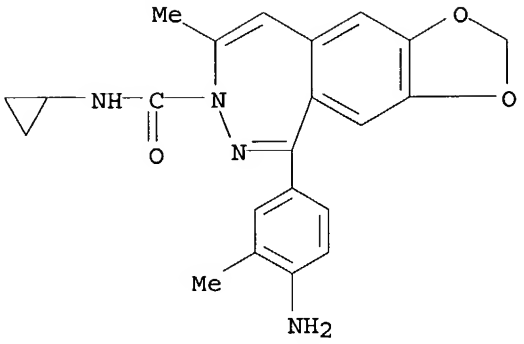
RN 319907-73-8 CAPLUS
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine, 7-acetyl-5-(4-amino-3-methylphenyl)-8-methyl- (9CI) (CA INDEX NAME)



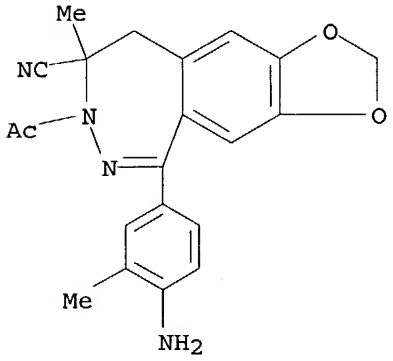
RN 319907-74-9 CAPLUS
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine-7-carboxamide, 5-(4-amino-3-methylphenyl)-N,8-dimethyl- (9CI) (CA INDEX NAME)



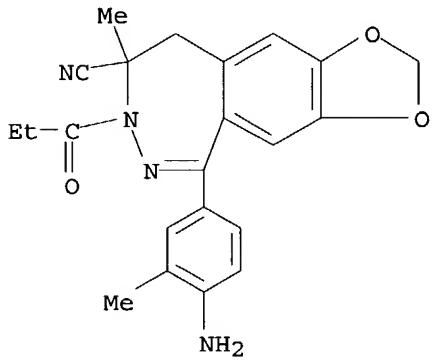
RN 319907-75-0 CAPLUS
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine-7-carboxamide, 5-(4-amino-3-methylphenyl)-N-cyclopropyl-8-methyl- (9CI) (CA INDEX NAME)



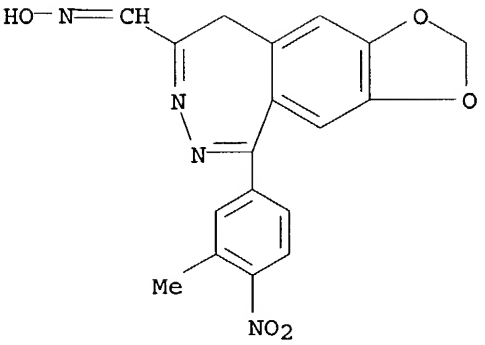
RN 319907-76-1 CAPLUS
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine-8-carbonitrile, 7-acetyl-5-(4-amino-3-methylphenyl)-8,9-dihydro-8-methyl- (9CI) (CA INDEX NAME)



RN 319907-77-2 CAPLUS
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine-8-carbonitrile, 5-(4-amino-3-methylphenyl)-8,9-dihydro-8-methyl-7-(1-oxopropyl)- (9CI) (CA INDEX NAME)



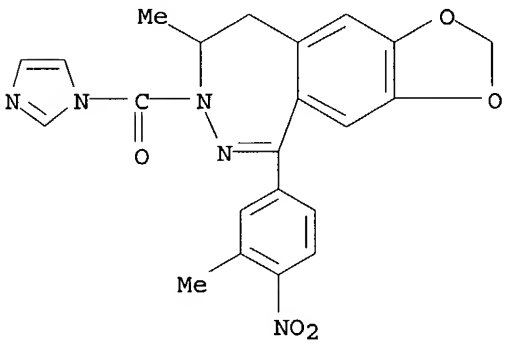
RN 319907-78-3 CAPLUS
CN 9H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine-8-carboxaldehyde, 5-(3-methyl-4-nitrophenyl)-, oxime (9CI) (CA INDEX NAME)



IT **319907-83-0P 319907-84-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of new 1,3-dioxolo[4,5-h][2,3]benzodiazepines as neuroprotective agents)

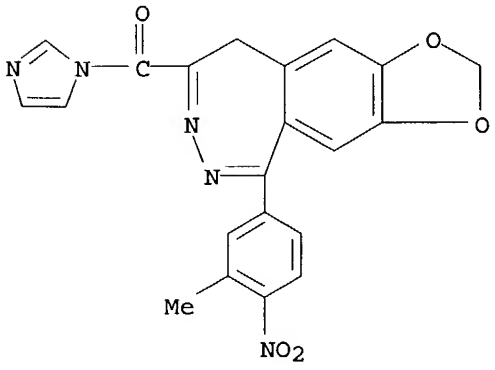
RN 319907-83-0 CAPLUS

CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine, 8,9-dihydro-7-(1H-imidazol-1-ylcarbonyl)-8-methyl-5-(3-methyl-4-nitrophenyl)- (9CI) (CA INDEX NAME)

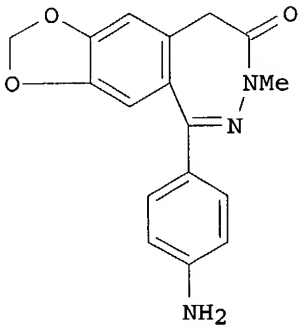


RN 319907-84-1 CAPLUS

CN 1H-Imidazole, 1-[[5-(3-methyl-4-nitrophenyl)-9H-1,3-dioxolo[4,5-h][2,3]benzodiazepin-8-yl]carbonyl]- (9CI) (CA INDEX NAME)



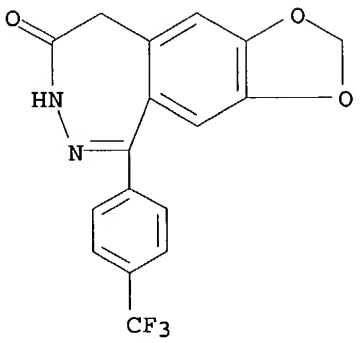
L20 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:348901 CAPLUS
DOCUMENT NUMBER: 131:102262
TITLE: Synthesis and anticonvulsant activity of new 2,3-benzodiazepines as AMPA receptor antagonists
AUTHOR(S): De Sarro, Angela; De Sarro, Giovambattista; Gitto, Rosaria; Grasso, Silvana; Micale, Nicola; Zappala, Maria
CORPORATE SOURCE: Cattedra di Chemioterapia, Istituto di Farmacologia, Facolta di Medicina, Universita di Messina, Messina, I-98100, Italy
SOURCE: Farmaco (1999), 54(3), 178-187
CODEN: FRMCE8; ISSN: 0014-827X
PUBLISHER: Elsevier Science S.A.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB Novel 1-aryl-3,5-dihydro-7,8-methylenedioxy-4H-2,3-benzodiazepin-4-ones (e.g., I) were prepared, and their anticonvulsant effects were evaluated by using various models of exptl. epilepsy. The seizures were evoked both by means of auditory stimulation in DBA/2 mice and by pentylenetetrazole or maximal electroshock in Swiss mice. Some of these compds. possess marked anticonvulsant properties in all tests employed. The compds. antagonize seizures induced by AMPA in analogy to the structurally related 1-(4-aminophenyl)-4-methyl-7,8-methylenedioxy-5H-2,3-benzodiazepine (GYKI 52466), a well known noncompetitive AMPA-receptor antagonist. On the other hand, these novel 2,3-benzodiazepines exhibit anticonvulsant properties that are not affected by flumazenil, but are reversed by aniracetam. In addition, when compared to GYKI 52466, the new compds. show a longer-lasting anticonvulsant activity and a lower toxicity. Structure-activity relationships offered an approach for designing more potent agents.

IT **231623-79-3P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and anticonvulsant activity of new 2,3-benzodiazepines as AMPA receptor antagonists)
RN 231623-79-3 CAPLUS
CN 8H-1,3-Dioxolo[4,5-h][2,3]benzodiazepin-8-one, 7,9-dihydro-5-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:231195 CAPLUS
DOCUMENT NUMBER: 130:267459
TITLE: Substituted 2,3-benzodiazepin-4-ones and the use thereof
INVENTOR(S): Xia, Haiji; Cai, Sui Xiong; Field, George; Lan, Nancy C.; Wang, Yan
PATENT ASSIGNEE(S): CoCensys, Inc., USA
SOURCE: U.S., 24 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

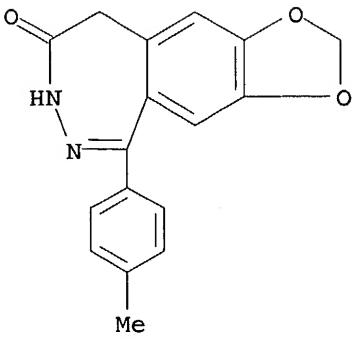
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5891871	A	19990406	US 1997-821638	19970320

PRIORITY APPLN. INFO.: US 1997-821638 19970320
OTHER SOURCE(S): MARPAT 130:267459

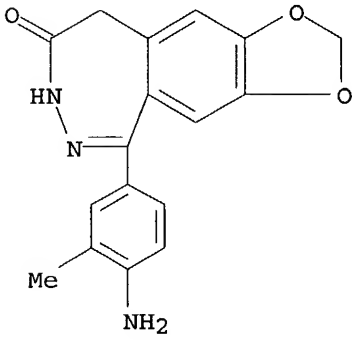
AB The invention relates to substituted 2,3-benzodiazepin-4-ones which are antagonists or pos. modulators of AMPA receptors, and the use thereof for treating, preventing or ameliorating neuronal loss associated with stroke, global and focal ischemia, CNS trauma, hypoglycemia and surgery, as well as treating or ameliorating neurodegenerative diseases including Alzheimer's disease, amyotrophic lateral sclerosis, Huntington's disease, Parkinson's disease and Down's syndrome, treating, preventing or ameliorating the adverse consequences of the overstimulation of the excitatory amino acids, treating or ameliorating anxiety, psychosis, convulsions, chronic pain, glaucoma, CMV retinitis, urinary incontinence, muscular spasm and inducing anesthesia, as well as for treating or ameliorating the adverse consequences of excitatory amino acid deficiency such as schizophrenia, Alzheimer's disease and malnutrition and neural maldevelopment, and as cognition enhancers. The invention also is directed to the process for the preparation of the substituted 2,3-benzodiazepin-4-ones. Thus, Me 4,5-methylenedioxy-2-(4-nitrobenzoyl)phenylacetate was cyclized with hydrazine to give 47% 7,8-methylenedioxy-1-(4-nitrophenyl)-3,5-dihydro-2,3-benzodiazepin-4(4H)-one, which was hydrogenated to give 73% 1-(4-aminophenyl)-7,8-methylenedioxy-3,5-dihydro-2,3-benzodiazepin-4(4H)-one which was derivatized, halogenated, acetylated, etc., to give approx. 70 title compds.

IT **197368-45-9P 197368-94-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and AMPA receptor activity of 2,3-benzodiazepin-4-ones)

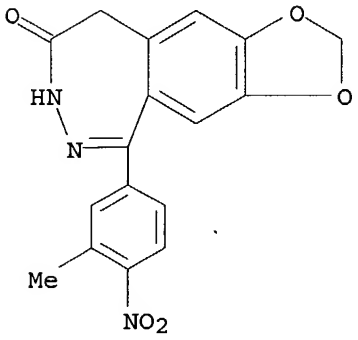
RN 197368-45-9 CAPLUS
CN 8H-1,3-Dioxolo[4,5-h][2,3]benzodiazepin-8-one, 7,9-dihydro-5-(4-methylphenyl)- (9CI) (CA INDEX NAME)



RN 197368-94-8 CAPLUS
CN 8H-1,3-Dioxolo[4,5-h][2,3]benzodiazepin-8-one, 5-(4-amino-3-methylphenyl)-7,9-dihydro- (9CI) (CA INDEX NAME)

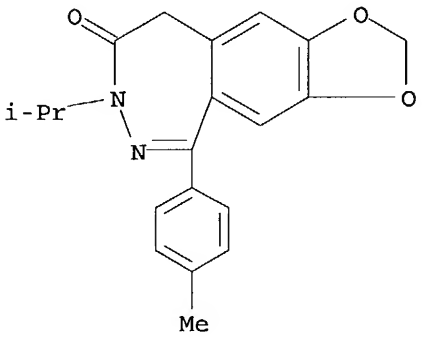


IT **197368-90-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and AMPA receptor activity of 2,3-benzodiazepin-4-ones)
RN 197368-90-4 CAPLUS
CN 8H-1,3-Dioxolo[4,5-h][2,3]benzodiazepin-8-one, 7,9-dihydro-5-(3-methyl-4-nitrophenyl)- (9CI) (CA INDEX NAME)



IT **197368-55-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and AMPA receptor activity of 2,3-benzodiazepin-4-ones)

RN 197368-55-1 CAPLUS
CN 8H-1,3-Dioxolo[4,5-h][2,3]benzodiazepin-8-one, 7,9-dihydro-7-(1-methylethyl)-5-(4-methylphenyl)- (9CI) (CA INDEX NAME)

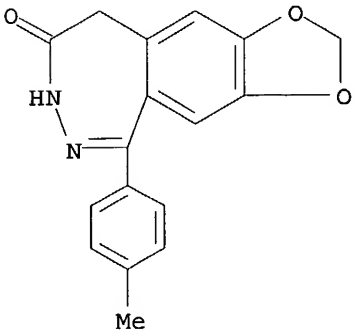


REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:429040 CAPLUS
DOCUMENT NUMBER: 129:109072
TITLE: Synthesis of 7,8-(methylenedioxy)-1-phenyl-3,5-dihydro-4H-2,3-benzodiazepin-4-ones as novel and potent noncompetitive AMPA receptor antagonists
AUTHOR(S): Wang, Yan; Konkoy, Christopher S.; Ilyin, Victor I.; Vanover, Kimberly E.; Carter, Richard B.; Weber, Eckard; Keana, John F. W.; Woodward, Richard M.; Cai, Sui Xiong
CORPORATE SOURCE: CoCensys Inc., Irvine, CA, 92618, USA
SOURCE: Journal of Medicinal Chemistry (1998), 41(14), 2621-2625
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A group of 7,8-(methylenedioxy)-1-phenyl-3,5-dihydro-4H-2,3-benzodiazepin-4-ones was synthesized and assayed for antagonism of rat brain α-amino-3-hydroxy-5-methylisoxazole-4-propionic acid (AMPA) receptors expressed in Xenopus oocytes. The benzodiazepinones inhibited AMPA-activated membrane current responses in a manner consistent with noncompetitive, allosteric inhibition of the receptor-channel complex. The most potent compound in the series was 1-(4-aminophenyl)-7,8-(methylenedioxy)-3,5-dihydro-4H-2,3-benzodiazepin-4-one (I), which had an IC50 of 2.7 μM. For comparison, the reference compound GYKI 52466 had an IC50 of 6.9 μM. I also had potent anticonvulsant activity in a mouse maximum electroshock-induced seizure (MES) assay: the ED50 was 2.8 mg/kg i.v., whereas the ED50 for GYKI 52466 was 4.6 mg/kg i.v. In contrast to a previous report, the 7,8-dimethoxy analog of I was a low-potency AMPA antagonist (IC50 >100 μM) and weak anticonvulsant (ED50 >10 mg/kg i.v.). The benzodiazepinones described herein are potent noncompetitive AMPA receptor antagonists that could have therapeutic potential as anticonvulsants and neuroprotectants.

IT **197368-45-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis of 7,8-(methylenedioxy)-1-phenyl-3,5-dihydro-4H-2,3-benzodiazepin-4-ones as AMPA receptor antagonists)
RN 197368-45-9 CAPLUS
CN 8H-1,3-Dioxolo[4,5-h][2,3]benzodiazepin-8-one, 7,9-dihydro-5-(4-methylphenyl)- (9CI) (CA INDEX NAME)



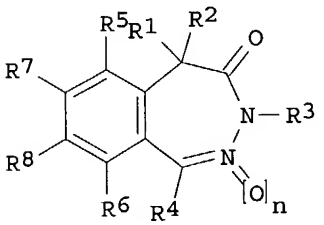
REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS

L20 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:640650 CAPLUS
DOCUMENT NUMBER: 127:307403
TITLE: Preparation of substituted 2,3-benzodiazepin-4-ones as antagonists or positive modulators of AMPA receptors
INVENTOR(S): Xia, Haiji; Field, George; Lan, Nancy C.; Wang, Yan; Cai, Sui Xiong
PATENT ASSIGNEE(S): Cocensys, Inc., USA; Acea Pharmaceuticals, Inc.; Xia, Haiji; Field, George; Lan, Nancy C.; Wang, Yan; Cai, Sui Xiong
SOURCE: PCT Int. Appl., 95 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9734878	A1	19970925	WO 1997-US3462	19970321
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9725270	A1	19971010	AU 1997-25270	19970321
JP 2000506890	T2	20000606	JP 1997-533496	19970321
EP 1021418	A1	20000726	EP 1997-916722	19970321
EP 1021418	B1	20040519		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
ZA 9702496	A	19971002	ZA 1997-2496	19970324

PRIORITY APPLN. INFO.: US 1996-13813P P 19960321
WO 1997-US3462 W 19970321

OTHER SOURCE(S): MARPAT 127:307403
GI



I

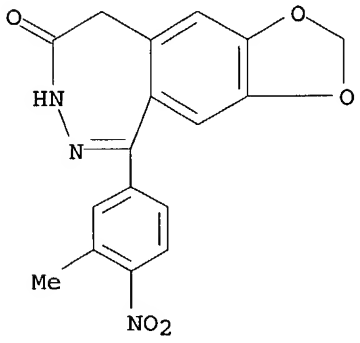
AB The title compds. [I; R1, R2 = H, alkyl, aryl, etc.; R1R2 = carbocycle, heterocycle; R3 = H, alkyl, haloalkyl, etc.; R4 = (un)substituted aryl, fused aryl, heteroaryl, etc.; R5, R6 = H, halo, haloalkyl, etc.; R7, R8 = H, halo, aryl, etc.; n = 0-1], useful for treating, preventing or ameliorating neuronal loss associated with stroke, global and focal ischemia, CNS trauma, hypoglycemia and surgery, as well as treating or ameliorating

neurodegenerative diseases including Alzheimer's disease, amyotrophic lateral sclerosis, Huntington's disease, Parkinson's disease and Down's syndrome, treating, preventing or ameliorating the adverse consequences of the overstimulation of the excitatory amino acids, treating or ameliorating anxiety, psychosis, convulsions, chronic pain, glaucoma, CMV retinitis, urinary incontinence, muscular spasm and inducing anesthesia, as well as for treating or ameliorating the adverse consequences of excitatory amino acid deficiency such as schizophrenia, Alzheimer's disease and malnutrition and neural maldevelopment, and as cognition enhancers, were prepared Thus, reaction of Me 4,5-methylenedioxy-2-(4-methylbenzoyl)phenylacetate with N2H4 and AcOH in EtOH afforded I [R1-R3 = H; R4 = 4-MeC6H4; R5-R6 = H; R7R8 = OCH2O; n = 0] which showed IC50 of 15 μM against AMPA receptors binding.

IT **197368-90-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of substituted 2,3-benzodiazepin-4-ones as antagonists or pos. modulators of AMPA receptors)

RN 197368-90-4 CAPLUS

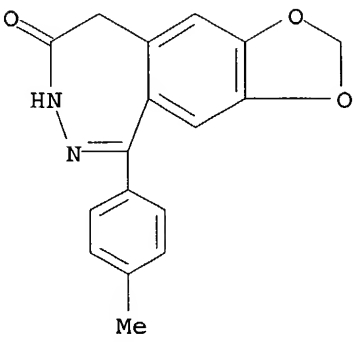
CN 8H-1,3-Dioxolo[4,5-h][2,3]benzodiazepin-8-one, 7,9-dihydro-5-(3-methyl-4-nitrophenyl)- (9CI) (CA INDEX NAME)



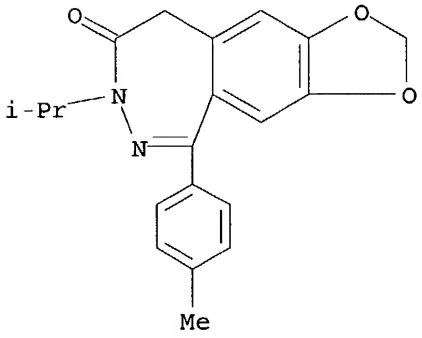
IT **197368-45-9P 197368-55-1P 197368-94-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted 2,3-benzodiazepin-4-ones as antagonists or pos. modulators of AMPA receptors)

RN 197368-45-9 CAPLUS

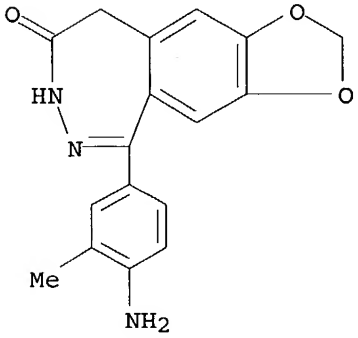
CN 8H-1,3-Dioxolo[4,5-h][2,3]benzodiazepin-8-one, 7,9-dihydro-5-(4-methylphenyl)- (9CI) (CA INDEX NAME)



RN 197368-55-1 CAPLUS
CN 8H-1,3-Dioxolo[4,5-h][2,3]benzodiazepin-8-one, 7,9-dihydro-7-(1-methylethyl)-5-(4-methylphenyl)- (9CI) (CA INDEX NAME)



RN 197368-94-8 CAPLUS
CN 8H-1,3-Dioxolo[4,5-h][2,3]benzodiazepin-8-one, 5-(4-amino-3-methylphenyl)-7,9-dihydro- (9CI) (CA INDEX NAME)

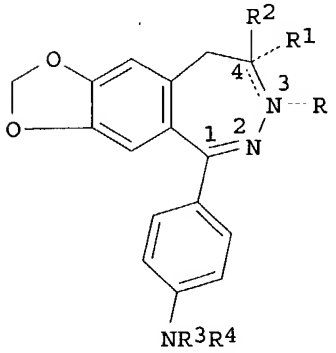


L20 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:366157 CAPLUS
DOCUMENT NUMBER: 125:114722
TITLE: N-Acyl 1-(4-aminophenyl)-4-methyl-7,8-methylenedioxy-2,3-benzodiazepine derivatives as excitatory amino acid antagonists useful as anticonvulsants, muscle relaxants, and neuroprotectants
INVENTOR(S): Andrasi, Ferenc; Berzsenyi, Pal; Botka, Peter; Farkas, Sandor; Goldschmidt, Katalin; Hamori, Tamas; Koroesi, Jeno; Moravcsik, Imre; Tarnawa, Istvan
PATENT ASSIGNEE(S): Gyogyszerkutato Intezet, Hung.
SOURCE: U.S., 22 pp., Cont.-in-part of U. S. Ser. No. 423,166.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5519019	A	19960521	US 1995-472454	19950607
HU 59684	A2	19920629	HU 1990-8398	19901221
HU 219778	B	20010730		
US 5459137	A	19951017	US 1993-80604	19930621

PRIORITY APPLN. INFO.:
HU 1990-8398 A 19901221
US 1991-809361 B2 19911217
US 1993-48347 B2 19930415
US 1993-80604 A3 19930621
US 1995-423166 A2 19950417

OTHER SOURCE(S): MARPAT 125:114722
GI



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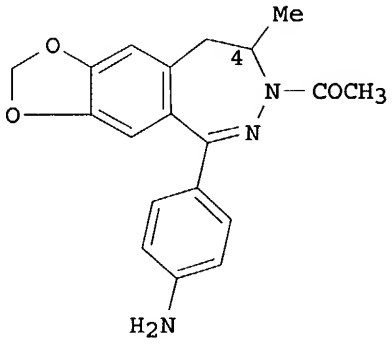


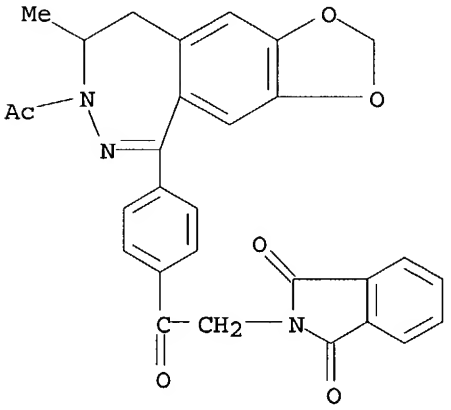
II

AB A method of blocking the activation of one or more excitatory amino acid receptors in mammals is claimed, which comprises administering to a mammal in need of decreased excitatory amino acid neurotransmission a pharmaceutically effective amount of a compound of formula I wherein R is a C1-6 alkanoyl group optionally substituted by a methoxy, cyano, carboxyl, amino, C1-4 alkylamino, di(C1-4 alkyl)amino, pyrrolidino, phthalimido or Ph group, or by one or more halogen(s); or R is a benzoyl, cyclopropanecarbonyl, C1-5 alkylcarbamoyl or phenylcarbamoyl group; or R is absent when a double bond exists between the N(3) and C(4) atoms; R1 is

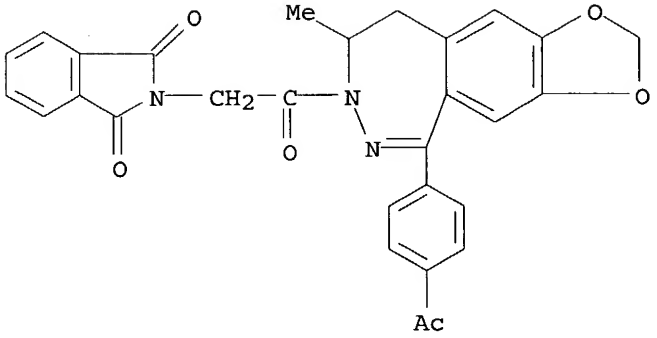
hydrogen, or R1 is absent when a double bond exists between the N(3) and C(4) atoms; R2 is a C1-3 alkyl group; or R1 and R2 together form a methylene group; R3 is hydrogen or a C1-4 alkanoyl group; R4 is hydrogen; a C1-6 alkanoyl group optionally substituted by a methoxy, cyano, carboxyl, amino, C1-4 alkylamino, di(C1-4 alkyl)amino, pyrrolidino, phthalimido or Ph group or by one or more halogen(s); as well as a benzoyl, palmitoyl, cyclopropanecarbonyl, C1-5 alkylcarbamoyl or phenylcarbamoyl group; with the proviso that no double bond exists between the N(3) and C(4) atoms when both R3 and R4 stand for hydrogen; and stereoisomers and pharmaceutically acceptable salts. Thus, e.g., acetylation of 1-(4-aminophenyl)-4-methyl-7,8-methylenedioxy-3,4-dihydro-5H-2,3-benzodiazepine with Ac2O afforded 85.7% 1-(4-aminophenyl)-3-acetyl-4-methyl-7,8-methylenedioxy-3,4-dihydro-5H-2,3-benzodiazepine (II) which exhibited inhibition of synaptic field potentials in rat hippocampal slices (an indicator of selective AMPA antagonist activity) with IC50 = 24.8 μM vs. 31.7 μM for GYKI 52466. Data are presented as well for the anticonvulsant, muscle-relaxant, and neuroprotective activity of I. Pharmaceutical formulations were given.

IT **179107-16-5P 179107-17-6P 179107-18-7P**
179107-19-8P 179107-20-1P 179107-21-2P
179107-22-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(N-acyl 1-(4-aminophenyl)-4-methyl-7,8-methylenedioxy-2,3-benzodiazepine derivs. as excitatory amino acid antagonists useful as anticonvulsants, muscle relaxants, and neuroprotectants)

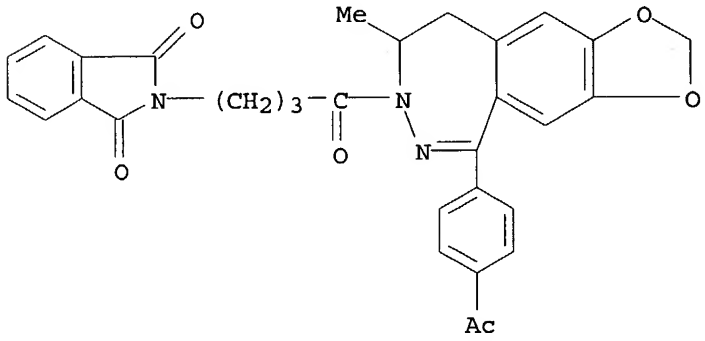
RN 179107-16-5 CAPLUS
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine, 7-acetyl-5-[4-[(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)acetyl]phenyl]-8,9-dihydro-8-methyl- (9CI) (CA INDEX NAME)



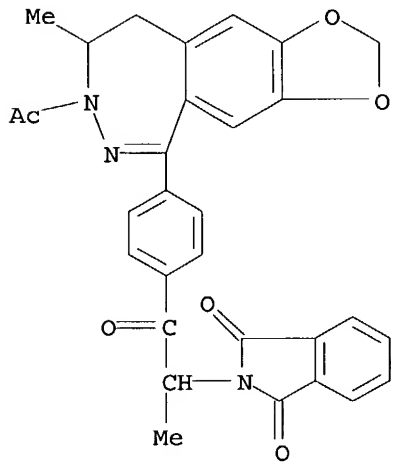
RN 179107-17-6 CAPLUS
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine, 5-(4-acetylphenyl)-7-[(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)acetyl]-8,9-dihydro-8-methyl- (9CI) (CA INDEX NAME)



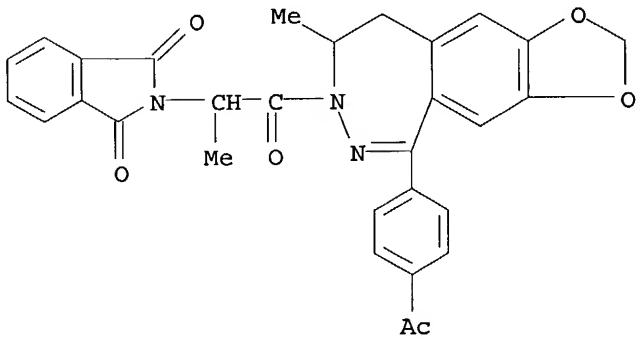
RN 179107-18-7 CAPLUS
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine, 5-(4-acetylphenyl)-7-[4-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)-1-oxobutyl]-8,9-dihydro-8-methyl- (9CI) (CA INDEX NAME)



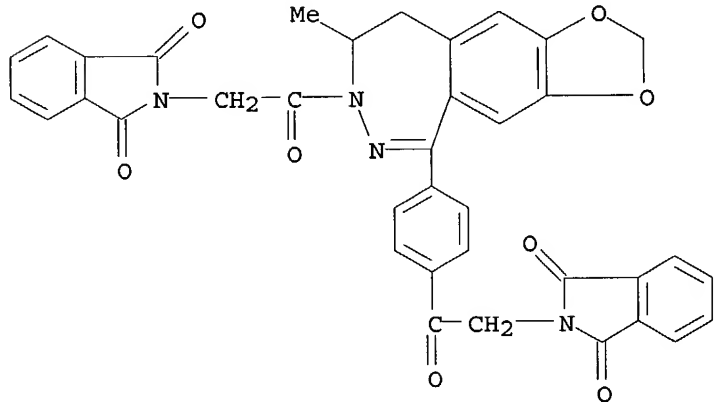
RN 179107-19-8 CAPLUS
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine, 7-acetyl-5-[4-[2-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)-1-oxopropyl]phenyl]-8,9-dihydro-8-methyl- (9CI) (CA INDEX NAME)



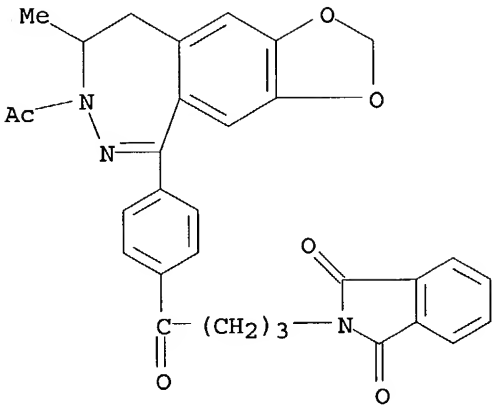
RN 179107-20-1 CAPLUS
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine, 5-(4-acetylphenyl)-7-[2-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)-1-oxopropyl]-8,9-dihydro-8-methyl- (9CI) (CA INDEX NAME)



RN 179107-21-2 CAPLUS
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine, 7-[(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)acetyl]-5-[4-[(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)acetyl]phenyl]-8,9-dihydro-8-methyl- (9CI) (CA INDEX NAME)



RN 179107-22-3 CAPLUS
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine, 7-acetyl-5-[4-[4-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)-1-oxobutyl]phenyl]-8,9-dihydro-8-methyl- (9CI) (CA INDEX NAME)


Me
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Ac
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N
O
C
(CH2)3
N
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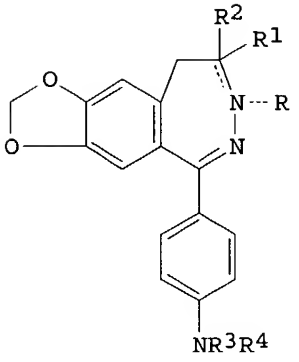
O

L20 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1992:571479 CAPLUS
DOCUMENT NUMBER: 117:171479
TITLE: Preparation of 1-(4-aminophenyl)-7,8-methylenedioxy-2,3-benzodiazepines as muscle relaxants, anticonvulsants, and cerebral antiischemics
INVENTOR(S): Andrasi, Ferenc; Berzsenyi, Pal; Botka, Peter; Farkas, Sandor; Goldschmidt, Katalin; Hamori, Tamas; Korosi, Jeno; Moravcsik, Imre; Tarnawa, Istvan
PATENT ASSIGNEE(S): Gyogyszerkutato Intezet, Hung.
SOURCE: Eur. Pat. Appl., 47 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 492485	A1	19920701	EP 1991-121882	19911223
EP 492485	B1	19971119		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
HU 59684	A2	19920629	HU 1990-8398	19901221
HU 219778	B	20010730		
CA 2057504	AA	19920622	CA 1991-2057504	19911212
CA 2057504	C	20020212		
BR 9105517	A	19920901	BR 1991-5517	19911219
RU 2102387	C1	19980120	RU 1991-5010635	19911219
FI 9106032	A	19920622	FI 1991-6032	19911220
NO 9105060	A	19920622	NO 1991-5060	19911220
AU 9189963	A1	19920625	AU 1991-89963	19911220
AU 641578	B2	19930923		
CN 1062730	A	19920715	CN 1991-111088	19911220
CN 1041420	B	19981230		
ZA 9110064	A	19921028	ZA 1991-10064	19911220
JP 05070463	A2	19930323	JP 1991-354972	19911220
JP 2756742	B2	19980525		
IL 100449	A1	19951231	IL 1991-100449	19911220
AT 160350	E	19971215	AT 1991-121882	19911223
ES 2112848	T3	19980416	ES 1991-121882	19911223
CN 1191111	A	19980826	CN 1998-103976	19980110
CN 1135980	B	20040128		

PRIORITY APPLN. INFO.: HU 1990-8398 A 19901221
OTHER SOURCE(S): MARPAT 117:171479
GI



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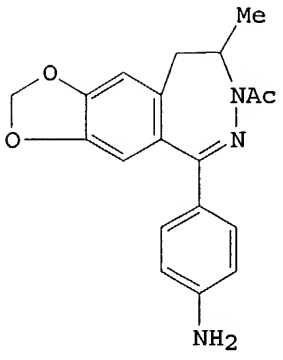


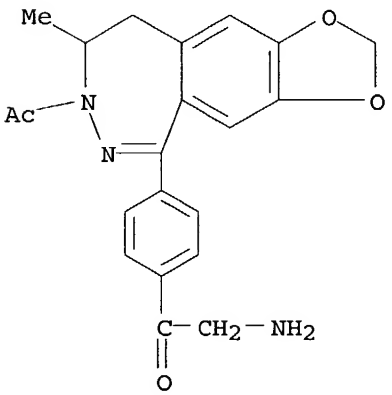
II

AB Title compds. [I; R = null, (substituted) aliphatic acyl, PhCO, cyclopropanecarbonyl, alkylcarbamoyl, phenylcarbamoyl; R1 = H, null; R2 = C1-3 alkyl; R1R2 = CH2; R3 = H, aliphatic acyl; R4 = H, (substituted) aliphatic acyl, PhCO, palmitoyl, cyclopropanecarbonyl, alkylcarbamoyl, phenylcarbamoyl; dotted lines = optional double bonds] were prepared Thus, 1-(4-aminophenyl)-4-methyl-7,8-methylenedioxy-3,4-dihydro-5H-2,3-benzodiazepine in CHCl3 was treated with Et3N and then Ac2O under ice cooling; the mixture was stirred 2 h to give 85.7% title compound II. II potentiated Na hexobarbital narcosis in mice with ED50 = 3-6 mg/kg orally, and inhibited electroshock-induced convulsion in mice with ED50 = 12.5 mg/kg orally. Tablets were prepared containing II.

IT **143691-92-3P 143691-98-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as muscle relaxant and anticonvulsant)

RN 143691-92-3 CAPLUS

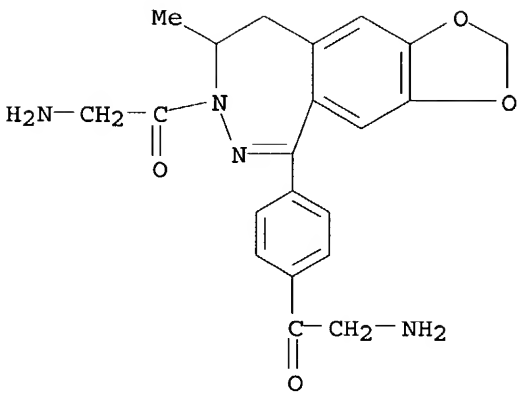
CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine, 7-acetyl-5-[4-(aminoacetyl)phenyl]-8,9-dihydro-8-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 143691-98-9 CAPLUS

CN 7H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine, 7-(aminoacetyl)-5-[4-(aminoacetyl)phenyl]-8,9-dihydro-8-methyl- (9CI) (CA INDEX NAME)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H2N—CH2—C
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C—CH2—NH2
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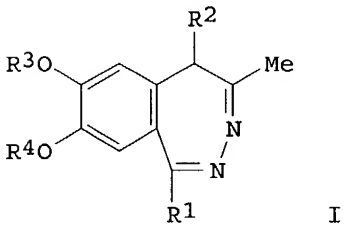
L20 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1986:533915 CAPLUS
DOCUMENT NUMBER: 105:133915
TITLE: 5H-2,3-benzodiazepines
INVENTOR(S): Lang, Tibor; Korosi, Jeno; Andrasi, Ferenc; Hamori, Tamas; Zolyomi, Gabor; Elekes, Istvan; Botka, Peter; Sineger, Eleonora; Goldschmidt, Katalin; et al.
PATENT ASSIGNEE(S): EGIS Gyogyszergyar, Hung.
SOURCE: Fr. Demande, 25 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2566774	A1	19860103	FR 1985-9793	19850627
FR 2566774	B1	19890317		
HU 37925	A2	19860328	HU 1984-2479	19840627
HU 191702	B	19870330		
ES 544633	A1	19860116	ES 1985-544633	19850627

PRIORITY APPLN. INFO.: HU 1984-2479 19840627
GI

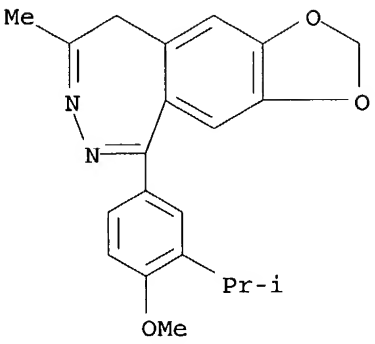


I

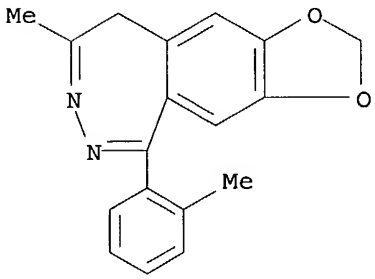
AB Title compds. I (R1 = Ph, furyl, naphthyl, thienyl, halo-, hydroxy-, or alkylphenyl, etc.; R2 = H, alkyl; R3 and R4 are alkyl or R3R4 = CH2) were prepared as antiaggressive agents. A 2-acetonylbenzophenone derivative was treated with N2H4 to give I (R1 = 3-ClC6H4, R2 = H, R3 = R4 = Me). In mice, selected I showed antiaggressive activity with ED50 of 16-50 mg/kg orally.

IT **104277-98-7P 104299-65-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as antiaggressive agent)

RN 104277-98-7 CAPLUS
CN 9H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine, 5-[4-methoxy-3-(1-methylethyl)phenyl]-8-methyl- (9CI) (CA INDEX NAME)



RN 104299-65-2 CAPLUS
CN 9H-1,3-Dioxolo[4,5-h][2,3]benzodiazepine, 5-(2-methylphenyl)-8-methyl-
(9CI) (CA INDEX NAME)



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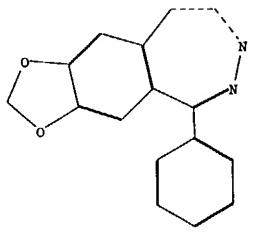
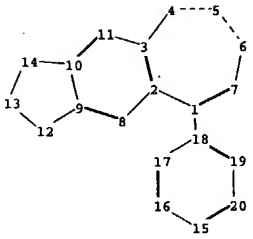
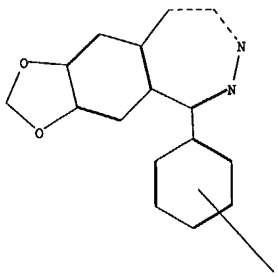


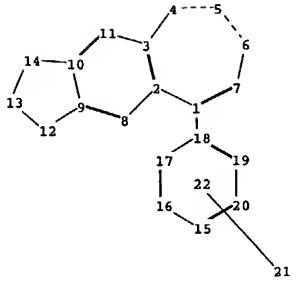


ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
chain bonds :
1-18
ring bonds :
1-2 1-7 2-3 2-8 3-4 3-11 4-5 5-6 6-7 8-9 9-10 9-12 10-11 10-14 12-13 13-14
15-16 15-20 16-17 17-18 18-19 19-20
exact/norm bonds :
1-2 1-7 3-4 4-5 5-6 6-7 9-12 10-14 12-13 13-14
exact bonds :
1-18
normalized bonds :
2-3 2-8 3-11 8-9 9-10 10-11 15-16 15-20 16-17 17-18 18-19 19-20

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom

C:\Program Files\Stnexp\Queries\10030436.str





chain nodes :
21
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
chain bonds :
1-18
ring bonds :
1-2 1-7 2-3 2-8 3-4 3-11 4-5 5-6 6-7 8-9 9-10 9-12 10-11 10-14 12-13 13-14
15-16 15-20 16-17 17-18 18-19 19-20
exact/norm bonds :
1-2 1-7 3-4 4-5 5-6 6-7 9-12 10-14 12-13 13-14
exact bonds :
1-18
normalized bonds :
2-3 2-8 3-11 8-9 9-10 10-11 15-16 15-20 16-17 17-18 18-19 19-20

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS
22:CLASS